Paper/Work

JULY 11, 2012
VOLUME 1, ISSUE 19

LAWRENCE LIVERMORE POSTDOC ASSOCIATION

POSTDOC ASSOCIATION INTERVIEW WITH DONA CRAWFORD

Dona Crawford is the LLNL Associate Director of Computation. She has been with the Lab since 2001 and is currently overseeing the implementation of Sequoia, the world's fastest supercomputer.

Dona met with the Postdoc Association for the fascinating and informative discussion that we present here. The following interview was conducted on May 15, 2012 by Adam Sorini and David Martinez. Photos and additional editing by Nathan Kugland.

David Martinez: Why did you decide to go to the national labs? After Stanford, did you go right to the national labs or did you do something in between?
Dona: My education and subsequent job search was a little more complicated than that. I earned a bachelor's degree in math and German, along with a teaching credential. I knew I could teach math but I was less confident in my German-speaking ability, so I got a master's degree in German. When I came back to the United States from Germany, there was a glut of teachers on the market. I needed to get a job, but it was not going to be teaching. I applied to organizations that might value both skills, including the intelligence agencies and the national laboratories. At the time, I was living in California, not too far from Sandia and Livermore labs. The response to my Livermore application was very slow; they asked me to come for an interview after I had accepted the job at Sandia. Sandia then paid for me to go to Stanford for a master's degree in operations research.

Adam Sorini: So you started off at Sandia? Could you talk about the first projects you worked on there?
Dona: I started as a numerical analyst. Based on my applied math education, I solved the first couple of problems in closed-form. My boss said, "That's interesting, but you can't do that all the time." I taught myself FORTRAN and wrote code to understand computing. Originally, I worked on non-linear PDEs for flame propagation inside internal combustion engines. In trying to make the code go faster, I became more familiar with the machine. Eventually, I ended up

POSTDOC ASSOCIATION INTERVIEW, CONTINUED

getting into operating systems and could make the computer run better by making tweaks there.

We had batch systems at the time—this is ancient history—and I remember when we got our first Cray with the Cray operating system (COS) in 1980. In the mid 1980s Sandia did a feasibility study to determine what it would take to move to the Cray Time Sharing System (CTSS). Many people at Sandia said we didn't have the resources to do this project, so my colleagues and I set out to prove them wrong. I worked closely with the Livermore CTSS experts and a small Sandia team, and we moved from COS to CTSS in only a few months. A couple of those Livermore experts are still here at the Lab. Shortly after that I became a first-level manager, overseeing all the operating systems in the Sandia/Livermore computing center.

Adam: What drew you to computer science?
Dona: I wanted to make the machine better. I saw (and still see) computers as incredible tools capable of everything from writing a symphony to understanding complex physical phenomena. But the computers weren't fast enough, and they weren't secure enough. You could overwrite memory, there were no checks on boundaries, and there were no access controls to compartmentalize information.

David: Why did you eventually come to LLNL?
Dona: I've always known that Livermore is the best place in the world for computing. It's the best in the world for two reasons: the great people who work here, and the fact that Livermore has computing in its blood. We were founded in September 1952, and by April 1953—just a few months later—we had our first supercomputer. This lab has always used computers as its tool of choice. In fact, the phrase "Simulation is the third leg of scientific discovery" was coined here. Yes, we have big computers, but more importantly we have the whole ecosystem to make those computers work well, including the best minds with the expertise and foresight to apply those computers to problems that make a difference in the world.

Adam: What about big data? Are we interested in that at Livermore?
Dona: Absolutely. Computation's R&D efforts focus on three goals: maintain a world-leading position in high performance computing, develop a Lab position in big data, and "broaden the base." Broadening the base has great value for both high performance computing and big data. In the last 15 years, we've started taking a hard look at data in terms of volume, variety, and velocity (the three Vs). We've been exploring the big data space with the intelligence community and in biosecurity fields. We also run the Earth System Grid, an international collaboration that collects climate science data from all over the globe. But, we haven't specifically identified our forcing function yet. During the next couple of years, I expect we'll fully flesh out a unifying big data goal and strategy for Livermore. What are the requirements at this lab? What unique expertise do we have? With whom should we partner? What architectures will be needed to support our efforts? What research needs to be done?

Adam: Big data seems like something that is en vogue lately. Obviously it's an important problem, but… maybe it'll go away.
Dona: I don't think so. The Earth System Grid of climate data is a few petabytes of data right now, but we expect to have 125 petabytes by 2020 and over 200 petabytes by 2025. How do you find the piece you want when networks run at 10 Gigabits per second? How are you going to transfer petabytes of data? The Large Synoptic Survey Telescope project uses a 3.2-gigapixel camera to take a picture of the night sky every 15 seconds. That's a tremendous amount of data being collected each night. Do you want to stream all that data down through a soda straw? What do you want to do with it? The accelerator at CERN has a similar problem with the data it's collecting. These are very real, complex problems that are not going away. In addition, smart meters,

POSTDOC ASSOCIATION INTERVIEW, CONTINUED

smart cities, social media – to name a few – are collecting more and more data every year. A recent UCSD report estimates the world generates a zettabyte of data a year and growing.

David: We've noticed that only five of the top ten supercomputers are in the United States, and none are here at Livermore (as of May 2012). Do you have any comments on that?
Dona: Our goal is to have the computing capability necessary to advance our mission. Our goal is not to be number one in the Top500 list. We're very proud when we're there because it is a measure, but it's not the measure. To rank in the Top500 requires running the LINPACK benchmark, which is Ax=b, a dense linear solver. It's not representative of our integrated codes and how we use a machine on a daily basis.

Having said that, the Top500 list is a way to compare machine architectures on a common problem. It shows that a system is up, stable, and firing on all cylinders for one calculation. It's also a matter of national pride. Some countries actually design their machines so they get the number one spot. Even though we didn't set out to have Sequoia be number one on the list, barring a big surprise it will be the most powerful machine in the world in terms of peak petaFLOPS. But, again, that's not our goal. [Editor's note: as of today, LLNL's Sequoia system is indeed #1 on the Top500 list.]

Adam: So, if we want time on Sequoia will we be able to get it?
Dona: There will be opportunities for science runs on Sequoia before it goes classified. We're running a set of benchmarks now, and we're running a Gordon Bell submission…

Adam: The one that we can't talk about?
Dona: The one we can't talk about. The fact that we're running a submission (several actually) is not a surprise, but we avoid discussing the details. Gordon Bell abstracts were turned in April 27, and full submissions were just submitted last week.

Adam: So have you run the LINPACK Benchmarks already?
Dona: We have.

Adam: What can you tell us about its performance?
Dona: We have all 96 racks on the floor, but the largest LINPACK run to date was on 72 racks, running at 76% efficiency. At half the machine, LINPACK ran at more than 80% efficiency, so we're confident we can optimize the system for an integrated full system LINPACK run.

Adam: Are postdocs important in the computational directorate?
Dona: The short answer is yes. Computer science requires a significant amount of research to advance the discipline, and our directorate's research and applications reach across a broad spectrum. Our PIs are involved in programmatic work, and they only have time to address the problem at hand. I'm delighted to have postdocs who are able to explore some longer-term concepts.

When I first came to Livermore, we had only five postdocs in Comp. There was a dot com boom in Silicon Valley, and it was hard enough to find someone who would get a PhD in computer science let alone pursue a postdoc position. Today, we have 21 postdocs in Computation. Given we have a little over 100 PhDs in the directorate, 21 postdocs is a good number. We want to make sure there are good projects and good mentors available for the postdocs. I'm proud that we've grown our postdoc population over the last 11 years. We benefit greatly from their ideas, enthusiasm, expertise, research, and publications.

Adam: Is it easier to keep them around now that the dot com boom is over?
Dona: We don't lose many postdocs to industry. It is more often the case they don't fit with the Lab culture or they want to fill out their resume before going to academia. The employees we lose to industry are staff employees with master's degrees or PhDs.

Adam: What do you do to try to keep them—pay them a lot more?
Dona: Money is always nice, but once you have enough to live on, it comes down to the work you do every day and why you do it. If money is your goal then you are better off going into industry. The people who come to

POSTDOC ASSOCIATION INTERVIEW, CONTINUED

the Lab want to make a difference and improve national security. And national security is not just about nuclear security; it's about our safety, our future, and our general way of living. People come here because they want to affect that.

I think if people don't stay it's because this was simply not the place for them, and that is okay. We've lost some employees to Twitter and Google; we see some of them regularly and establish collaborations. Comp tends to lose more people than the rest of the Lab to "better opportunities." We certainly can't compete with the big stock options that industry offers. If you have suggestions on how we can retain people, I'd love to hear them.

Adam: I think there is a GPU (Graphical Processing Unit) machine here and I was wondering if you have any comments on GPU computing for scientific research.
Dona: LLNL has always used GPUs for scientific visualization and in fact one of our "viz" clusters is currently #185 on the Top500 list. The question is how effectively we can harness GPUs for more general-purpose computing, turning GPUs into GPGPUs. We have some code teams that are enthusiastically embracing GPGPUs and are achieving promising results. Others are more wary, especially when it comes to investing time and effort to write proprietary CUDA code that is not portable to other platforms. We will continue to invest effort exploring GPUs and other accelerators such as Intel MIC, recognizing that flops per watt is an increasingly important metric for the power-hungry supercomputers of the future. We have an exploratory test bed so we can stay current with the latest technologies, including flash memory, transactional memory, speculative processing, and GPUs. We always have to know what's out there, and GPUs are getting more interesting.

David: Who are the biggest users for high performance computing besides the United States government, such as what type of industries?
Dona: The Fortune 100 companies use big computers: the oil and gas industries, the aeronautical industry, the automotive companies. They don't use them to the extent we do nor do they seek to push the bleeding edge the way we do, so we partner with them.

You would expect that companies like Boeing, Ford, GM, and the nuclear industry would be using high performance computing, and they do. But there are also some everyday products that are developed with high performance computing. For instance, Proctor and Gamble is an interesting user of HPC. They produce a large number of Pringles potato chips per hour, and they want to know how fast potato chips can move down the conveyer belt before the chips fly off like an airfoil. So they do the same calculations for a potato chip as the aeronautics or aerospace industry would do for an air wing. They also use computers to optimize the Pringles cans. They want to keep the weight of the cans low while maintaining durability, so they're not crushed when they're stacked and transported.

The pharmaceutical sector is starting to use more HPC for their research interests. If these companies can figure out how to reduce the number of drug trials by using computers, they would save billions of dollars.

Recently at the Lab, we've focused on working with energy companies, carbon capture companies, and shale gas fracking companies, utility companies, combustion companies. We're also partners in the Energy Efficiency Buildings Hub. The light bulbs at my home are not a big deal, but if you add up the light bulbs of 300 million homes and offices, and all the streetlights, it accounts for about 40% of the U.S. energy consumption. Unfortunately a large part of that is rejected or wasted energy. The Lab produces energy flow charts (https://flowcharts.llnl.gov/), which show the energy sources and where it goes in the United States. Increasing the efficiency of buildings would mean big savings.

On behalf of the Newsletter Team, thank you, Dona.

POSTDOC HIGHLIGHTS: NOTES TO THE DIRECTOR

X-ray vision exposes aerosol structures in *Nature*

LLNL researchers and international collaborators have peered into the makeup of complex airborne particulate matter so small that it can be transported into human lungs — usually without a trace. The structure of micron-size particles is important in a wide range of fields from toxicology to climate science; however, their properties are surprisingly difficult to measure in their native environment. Electron microscopy requires the collection of particles on a substrate and the analysis time makes it impractical to image numerous particles; visible light scattering provides insufficient resolution; and x-ray studies have, to date, been limited to ensembles of many particles. In the June 27 edition of *Nature*, researchers, including LLNL authors **Mark Hunter** (postdoc), George Farquar, W. Henry Benner, Stefan Hau-Riege, and Matthias Frank, report on an in situ method for imaging individual sub-micron particles to nanometer resolution in their native environment, using intense, coherent X-ray pulses from the Linac Coherent Light Source (LCLS) free-electron laser. The team, led by former LLNL postdoc (now at SLAC) **Mike Bogan**, introduced individual aerosol particles into the pulsed X-ray beam, which is sufficiently intense that diffraction from individual particles can be measured for morphological analysis. At the same time, ion fragments ejected from the beam were analyzed using mass spectrometry to determine the composition of individual particles. The aerosol particle injection technique used for this experiment was based LLNL's previous work on aerosol mass spectrometry. The results show the extent of internal symmetry of individual soot particles and a large variability in their fractal dimensions. This method, which can rapidly determine the morphology of large numbers of individual particles in a heterogeneous sample, can be applied to determine both the static and dynamic morphologies of other types of particles, and could help address questions such as solvent accessibilities in proteins, energy transfer by the hydrodynamic interaction of amino acids, and large-scale production of nanoscale structures by flame synthesis.
http://www.nature.com/nature/journal/v486/n7404/full/nature11222.html

New theory of surface-mediated spinodal decomposition

Spinodal decomposition is a widely occurring phase separation phenomenon that has an important influence on material behavior. It has been known for decades that the spinodal temperature, below which spinodal decomposition can develop, can be significantly suppressed in bulk crystalline systems, sometimes to several hundred kelvins, by the internal stress that results from the misfit between the different lattices of the phases in the spinoidal mixture. However, LLNL researcher **Ming Tang** (former postdoc) recently discovered from numerical simulations that spinodal decomposition can begin near free surfaces of a material, and then propagate into the interior of a crystal even at temperatures above the bulk spinodal temperature. In a paper published in the June 29, 2012 issue of *Physical Review Letters*, Tang and Alain Karma at Northeastern University explain this surprising finding in terms of general linear stability theory, and show that unlike the bulk-mode decomposition, misfit stress has no effect on the onset temperature of surface-mode spinodal decomposition because of stress relaxation near the free surface. Consequently, the unstable region on the phase diagram of a phase-separating crystal can be much larger when free surfaces are present. This finding sheds light on existing experimental observations, and has far- reaching implications for predicting and manipulating the stability of many technologically important materials, such as nanostructured Li-ion battery electrodes and III-V semiconductor thin films. In addition, surface-mode decomposition produces novel nanoscale structures that may find potential applications in nanopatterning and photoluminescence.
http://link.aps.org/doi/10.1103/PhysRevLett.108.265701

NOTES FROM THE LLPA COUNCIL MEETING ON JULY 5

Start: 7/5/2012, 12pm, B543 Good Earth room
Participants: Nathan Kugland, David Alessi, David Martinez, Kris Kulp, Kirsten Howley, Eric Wang, Eric Gard (LDRD), Abhinav Bhatele, Sarah Felix, Andre Schleife, Mandoye Ndoye, Charles Reid, Kyle Lang, Andy Pascal, Christine Zachow, Lance Simms, Geoffrey Feld

Introduction:
* $198 left in the Postdoc account (Nathan)
* Google Drive is current home for How-To documents, long-term solution still to find

BBQ-Picnic:
* more sales next week
* only 15 tickets sold by now, more publicity needed
* draft an email "Picnic in a week - why should you go?": include pictures, personal anecdotes, networking opportunities (Eric)
* invite summer students+advisors: send out to email list/Google group (Christine)

Outings:
* Karaoke night was awesome and will be repeated
* Euro 2012 viewing was fun, maybe more sport lunches during the Olympics

Web Team:
* lab decided on template
* will have the template soon and can start working with it
* Charles will help, needs access (Christine)
* Council will review current web page and makes suggestions, Abhinav assigns the individual pages to people from the Council (Abhinav)

Poster Symposium:
* planning will happen later, help will be needed
* call Tap 25 (Andre)
* print flyers to advertise the Happy Hour after the event (Andre)

Lab-wide LDRD issues:
Kyle presents his concerns:
* 106 proposals have been submitted (21 Engineering, 2 Comp, 5 NIF)
* 26 short-listed (no Eng., no Comp.) --> biased?
* divergence from what is presented at LDRD info sessions and actual experience
Eric replies:
* 25% of LDRD committee are engineers
* short-list was created without looking at whether PI is engineer or not
* each reviewer indicates his knowledge level for each of the proposals
* 3 reviewers are assigned per proposal to downselect
* criteria: merit (75%) and broader impact (25%)
* if there is a bias, it is unintentional, but the concern is acknowledged
* a session (maybe brown bag) is to be scheduled to discuss with the Postdoc community in mid/late August

Newsletter:
* Donna Crawford interview completed
* first contact with Ed Moses
* more staff needed (advertise at Poster Symposium and BBQ-Picnic)
* possible candidates for exit interviews: Cedric, Lance
* feature article that summarizes recent outings (Andre)

Career development:
* no contact could be made with Stanford yet
* try again (Nathan, Andre)

Director's Brown Bag:
* rescheduled due to complications

Closing remarks:
* Eric Gard emphasizes how well the work of the council is perceived, in particular the newsletter
* more help needed to keep up good work

COMMENTS/SUGGESTIONS/PRAISE/COMPLAINTS?

Please send your feedback to the Editor (Nathan Kugland, kugland1@llnl.gov).

CAREER RESOURCES

Upcoming events:

July 17, 2:30-5:30 pm:
5th Annual Institutional Postdoc Poster Symposium.
Register here: https://symposium.llnl.gov/postdoc

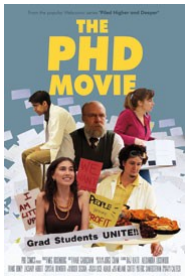
July 24, 11 am – 12 pm:
PLS postdoc seminar series
B151 R1209 (Stevenson Room)
Dina Weilhammer, BBTD
Bryan Hudson, BBTD

Writing a proposal?
Check out the Proposal Toolkit from the Office of Strategic Outcomes!

PROPOSAL TOOLKIT

https://oso-int.llnl.gov/imo/proposalToolkit-top.php

PILING ON



Several months ago, members of the LLNL community had the opportunity to see Jorge Cham's independent film, "The PhD Movie," based on his popular comic strip. This movie explored the existential question many graduate students face: Why am I doing this?

For most of us, the answer is that, despite the late nights, failed experiments, and endless grant writing, we are passionate about a career in science. In an article in *Nature*, however, Mariano Loza-Coll states that this film should serve as a wake-up call, arguing that we should change a culture which values a person's willingness to sacrifice their own personal fulfillment.

"It is not scientists, but the rest of society that may suffer most if scientists end up burning out. To ensure that scientists can cure diseases, feed the hungry and prevent environmental catastrophes, we should select them on the basis of their intelligence, effectiveness and focus, not their personal sacrifices, obsession and stamina."

MOTIVATING SCIENTISTS

Adapted from **Motivate Your Lab**, by Edyta Zielinska
Published in **The Scientist,** June 2012

As postdocs, a goal of many of us is to manage our own lab or group. Such management is no easy task, and is not one for which scientists are usually explicitly trained. Below are some pointers on ways to lead a team to glorious scientific victory.

Define the motivation. Discern how best to motivate each team member. Some people are better at avoidance goals. Some are better at approach goals. Find them out, and you can frame tasks as either gaining a positive goal or avoiding a negative one.
Diagnose lack of motivation. At times managers will perceive a lack of motivation or progress from a particular team member. They may feel that their goal is not valued, is unattainable, or may feel weighed down by micromanagement. Determining this root cause can improve progress toward the goal.
Encourage mistakes. Perfectionism can lead to myopia and to not searching widely for solutions. We may emphasize perfection too much, at the expense of success – in short: fail fast, often, and cheaply.
Get uncomfortable. When a person can focus at least a part of each day on the uncomfortable things that he or she is not good at, it usually leads to tremendous improvement over time.
Spur creativity. Have your team members try to solve a problem under new constraints. What might a competitor's lab do; what would a lab with few or many resources do? Imagining the problem in a different context can help people relax their assumptions.

JOB LINKS

Science Careers naturejobs.com The premier science jobs recruitment website

Science Careers – Featured jobs:
http://scjobs.sciencemag.org/featured-jobs/
Nature – Jobs of the week:
http://www.nature.com/naturejobs/science/
Official LLNL jobs site: careers.llnl.gov
Postdoc listings: www.postdocjobs.com
Academic jobs: www.academickeys.com
APS Careers in Physics: www.aps.org/careers
Government jobs: www.usajobs.gov/
Industry jobs: www.indeed.com
www.monster.com
sfbay.craigslist.org/jjj/
www.linkedin.com/jobs

SELECTED RECENT POSTDOC RESEARCH PUBLICATIONS

Bold = LLNL Postdoc. *Broadcast your achievements! Make new connections & help show how we are doing collectively.*

Guidelines: 1) Peer-reviewed and accepted publications (journal or conference proceedings) only; 2) Your affiliation must be LLNL; 3) Prepare a standard-format citation with all authors (no *et al*), the full title, journal/proceedings info, and a link to the online abstract; 4) Note which authors are LLNL postdocs, and in what division & group; 5) Send all of this to Nathan (kugland1@llnl.gov).

WCI/AX Division/Asteroid Group: Dorman, Claire E., Guhathakurta, Puragra, Fardal, Mark A., Lang, Dustin, Geha, Marla C., **Howley, Kirsten M.**, Kalirai, Jason S., Bullock, James S., Cuillandre, Jean-Charles, Dalcanton, Julianne J., Gilbert, Karoline M., Seth, Anil C., Tollerud, Erik J., Williams, Benjamin F., Yniguez, Basilio, "The SPLASH Survey: Kinematics of Andromeda's Inner Spheroid," The Astrophysical Journal, 752, 147 (2012) http://dx.doi.org/10.1088/0004-637X/752/2/147

PLS/BBTD (Koziol) and PLS/CSD (Floyd): **Koziol L**, Valdez CA, Baker SE, Lau EY, **Floyd WC 3rd**, Wong SE, Satcher JH Jr, Lightstone FC, Aines RD, "Toward a Small Molecule, Biomimetic Carbonic Anhydrase Model: Theoretical and Experimental Investigations of a Panel of Zinc(II) Aza-Macrocyclic Catalysts" Inorg Chem. 2012 Jun 18;51(12):6803-12. Epub 2012 Jun 6. http://pubs.acs.org/doi/abs/10.1021/ic300526b

PLS/Chemical Sciences Division/Chemical and Isotopic Signatures Group:

Wilson, R. L., J. F. Frisz, W. P. Hanafin, **K. J. Carpenter**, I. D. Hutcheon, P. K. Weber, and M. L. Kraft. "Fluorinated colloidal gold immunolabels for imaging select proteins in parallel with lipids using high-resolution secondary ion mass spectrometry." *Biconjugate Chemistry*, 23: (3) 450, 2012 http://pubs.acs.org/doi/abs/10.1021/bc200482z

Carpenter, K. J., A. Horak, L. Chow, and P. J. Keeling. "Symbiosis, morphology, and phylogeny of Hoplonymphidae (Parabasalia) of the wood-feeding roach *Cryptocercus punctulatus*." *Journal of Eukaryotic Microbiology*, 58: 426, 2011. (COVER). http://onlinelibrary.wiley.com/doi/10.1111/j.1550-7408.2011.00564.x/abstract

Gile, G., E. James, R. Scheffrahn, **K. J. Carpenter**, and Patrick J. Keeling. "Molecular and morphological analysis of the Calonymphidae with a description of *Calonympha chia* sp. nov., *Snyderella kirbyi* sp. nov., and *Snyderella swezyae* sp. nov. *International Journal of Systematic and Evolutionary Microbiology*, 61: 2547, 2012. (COVER) http://ijs.sgmjournals.org/content/61/10/2547.abstract

PLS/CMMD/High Performance Computational Materials Science and Chemistry Group: **A. Stukowski**, "Structure identification methods for atomistic simulations of crystalline materials," *Modelling Simul. Mater. Sci. Eng.* **20** (2012)**,** 045021 http://dx.doi.org/10.1088/0965-0393/20/4/045021

LLNL POSTDOC ASSOCIATION LEADERSHIP COUNCIL

President Nathan Kugland
Vice President Andre Schleife
Handbook Editor Mandoye Ndoye
Newsletter Team
David Alessi, Nick Be, David Martinez, Nathan Kugland
Web Team: Abhinav Bhatele, Charles Reid, Mandoye Ndoye
Social Events Team: Kirsten Howley, Andre Schleife
Career Development Team: Nick Be
Participating Councilmembers:
Lance Simms, Liam Stanton, Eric Wang, Heather Whitley
LLNL Postdoc Advisory Committee Staff Representatives
Kris Kulp, Christine Zachow